LISTING OF AND AMENDMENTS TO CLAIMS:

1. (currently amended) A method for obtaining at least one calibration filter for a Mass Spectrometry (MS) instrument system, comprising the steps ~~step~~ of:

obtaining, for a given calibration ion with its isotopes, measured isotope peak cluster data in a mass spectral range;

calculating, for the given calibration ion with its isotopes, relative isotope abundances and actual mass locations of isotopes corresponding thereto;

specifying mass spectral target peak shape functions;

performing convolution operations between the calculated relative isotope abundances and the mass spectral target peak shape functions to form calculated isotope peak cluster data; and

performing a deconvolution operation between the measured isotope peak cluster data and the calculated isotope peak cluster data after the convolution operations to obtain the at least one calibration filter.

2. (original) The method of claim 1, wherein any of said steps of performing convolution operations and performing a deconvolution operation employs at least one of a Fourier Transform, a matrix multiplication, and a matrix inversion.

3. (original) The method of claim 1, further comprising the step of pre-aligning measured mass spectral isotope peaks based on a least squares fit between centroid masses of the calculated relative isotope abundances and those of the measured isotope peak clusters, in a pre-calibration step performed subsequent to said calculating step.

4. (original) The method of claim 1, further comprising the steps of:

performing pre-calibration instrument-dependent transformations on raw mass spectral data; and

performing post-calibration instrument-dependent transformations on a calculated data set corresponding to a test sample.

5. (original) The method of claim 4, wherein said steps of performing pre-calibration instrument-dependent transformations and performing post-calibration instrument-dependent transformations involve respectively creating a pre-calibration banded diagonal matrix and a post-calibration banded diagonal matrix, each nonzero element along a banded diagonal of each of the respective matrices for respectively performing an interpolation function corresponding to the pre-calibration instrument-dependent transformations and the post-calibration instrument-dependent transformations, and said method further comprises the step of creating from the at least one calibration filter a calibration banded diagonal matrix for performing both peak shape and mass axis calibration.

6. (original) The method of claim 5, further comprising the step of multiplying the pre-calibration banded diagonal matrix, the calibration banded diagonal matrix and the post-calibration banded diagonal matrix into a total filtering matrix prior to calibrating a test sample.

7. (original) The method of claim 6, wherein the peak shape and the mass axis calibration are performed by matrix multiplication between the total filtering matrix and the raw mass spectral data, and said method further comprises the step of creating another banded diagonal matrix to estimate mass spectral variances of a calibrated signal, the other banded diagonal matrix having each nonzero element along a banded diagonal equal to a square of a corresponding element in the total filtering matrix.

8. (original) The method of claim 7, further comprising the step of applying a weighted regression operation to calibrated mass spectral data to obtain at least one of integrated peak areas, actual masses and other mass spectral peak data for the mass spectral peaks.

9. (original) The method of claim 8, wherein weights of the weighted regression operation are proportional to an inverse of the mass spectral variances.

10. (original) The method of claim 7, further comprising the step of applying multivariate statistical analysis to calibrated mass spectral data to at least one of quantify, identify, and classify test samples.

11. (original) The method of claim 1, further comprising the steps of:

performing a pre-calibration mass spacing adjustment from a non-uniformly spaced mass acquisition interval to a uniformly spaced mass interval; and

performing a post-calibration mass spacing adjustment from the uniformly spaced mass interval to a reporting interval.

12. (original) The method of claim 11, wherein said steps of performing the pre-calibration mass spacing adjustment and the post-calibration mass spacing adjustment involve respectively creating a pre-calibration banded diagonal matrix and a post-calibration banded diagonal matrix, each nonzero element along a banded diagonal of each of the respective matrices for respectively performing an interpolation function corresponding to the pre-calibration mass spacing adjustment and the post-calibration mass spacing adjustment, and said method further comprises the step of creating from the at least one calibration filter a calibration banded diagonal matrix for performing both peak shape and mass axis calibration.

13. (original) The method of claim 12, further comprising the step of multiplying the pre-calibration banded diagonal matrix, the calibration banded diagonal matrix and the post-calibration banded diagonal matrix into a total filtering matrix prior to calibrating a test sample.

14. (original) The method of claim 13, wherein the peak shape and the mass axis calibration are performed by matrix multiplication between the total filtering matrix and raw mass spectral data, and said method further comprises the step of creating another banded diagonal matrix to estimate mass spectral variances of a calibrated signal, the other banded diagonal matrix having each nonzero element along a banded diagonal equal to a square of a corresponding element in the total filtering matrix.

15. (original) The method of claim 14, further comprising the step of applying a weighted regression operation to calibrated mass spectral data to obtain at least one of integrated peak areas, actual masses and other mass spectral peak data for the mass spectral peaks.

16. (original) The method of claim 15, wherein weights of the weighted regression operation are proportional to an inverse of the mass spectral variances.

17. (original) The method of claim 14, further comprising the step of applying multivariate statistical analysis to calibrated mass spectral data to at least one of quantify, identify, and classify test samples.

18. (original) The method of claim 1, wherein the at least one calibration filter comprises at least two calibration filters, and said method further comprises the step of further interpolating between the at least two calibration filters to obtain at least one other calibration filter within a desired mass range.

19. (original) The method of claim 18, wherein said interpolating step comprises the steps of:

collecting the at least two calibration filters as vectors in a matrix for decomposition;

decomposing the matrix that includes the at least two calibration filters;

interpolating between decomposed vectors of the matrix to obtain interpolated vectors; and

reconstructing the at least one other calibration filter using the interpolated vectors.

20. (original) The method of claim 19, wherein said decomposing step is performed using at least one of Singular Value Decomposition (SVD) and wavelet decomposition.

21. (previously presented) The method of claim 1, further comprising the step of introducing the calibration standard one of prior to and in real-time through at least one of continuous infusion and online mixing so as to acquire both calibration data and test data in a single experiment.

22. (currently amended) A method of processing raw mass spectral data, comprising the steps of:

applying a total filtering matrix to the raw mass spectral data to obtain calibrated mass spectral data,

wherein the total filtering matrix is formed by:

measured isotope peak cluster data, obtained for a given calibration ion in a mass spectral range,

relative isotope abundances and actual mass locations of isotopes corresponding thereto, calculated for a same calibration ion,

specified mass spectral target peak shape functions,

convolution operations performed between the calculated relative isotope abundances and the mass spectral target peak shape functions to form calculated isotope peak cluster data; and

a deconvolution operation performed between the measured isotope peak cluster data and calculated isotope peak cluster data after the convolution operations to obtain at least one calibration filter for the total filtering matrix.

23. (original) The method of claim 22, wherein said applying step further comprises the step of interpolating the raw mass spectral data onto a same mass axis as that required by the total filtering matrix.

24. (original) The method of claim 22, wherein said applying step further comprises the step of interpolating the calibrated mass spectral data onto any desired mass axis different from that given by the total filtering matrix.

25. (original) The method of claim 22, further comprising the step of applying a weighted regression operation to the calibrated mass spectral data to obtain at least one of integrated peak areas, actual masses and other mass spectral peak data for the mass spectral peaks.

26. (original) The method of claim 25, wherein weights of the weighted regression operation are proportional to an inverse of mass spectral variances.

27. (original) The method of claim 22, further comprising the step of applying multivariate statistical analysis to the calibrated mass spectral data to at least one of quantify, identify, and classify test samples.

28. – 109. (canceled)

110. (previously presented) For use in a mass spectrometer having associated therewith a computer for performing data analysis functions of data produced by the mass spectrometer, a computer readable medium having placed thereon computer readable program instructions for performing the method of claim1.

111. (canceled).

112. (currently amended) A mass spectrometer having associated therewith a computer for performing data analysis functions of data produced by the mass spectrometer, the computer performing the method of ~~claim~~ any one of claims 1 - 27.

113. (canceled)

114. (previously presented) The method of claim 1, wherein said calibration filter, when applied to a mass spectrum, performs at least one of noise filtering, signal averaging, mass calibration, and peak shape adjustment.

115. (previously presented) For use in a mass spectrometer having associated therewith a computer for performing data analysis functions of data produced by the mass spectrometer, a computer readable medium having placed thereon computer readable program instructions for performing the method of claim 22.

116. (previously presented) A mass spectrometer having associated therewith a computer for performing data analysis functions of data produced by the mass spectrometer, the computer performing the method of claim 22.

117. (new) The method of claim 22, wherein said calibration filter is a linear filter and its application to raw mass spectral data involves one of convolution, matrix multiplication, or point-by-point multiplication through Fourier transformation.

118. (new) The method of claim 1, wherein said calibration filter is a digital filter.